

Abstract Submitted
for the DPP13 Meeting of
The American Physical Society

Energetics and Dynamics of Mobile Helium Clusters in Near-Surface Regions of Plasma-Exposed Tungsten LIN HU, Department of Chemical Engineering, University of Massachusetts, Amherst, KARL HAMMOND, BRIAN WIRTH, Department of Nuclear Engineering, University of Tennessee, Knoxville, DIMITRIOS MAROUDAS, Department of Chemical Engineering, University of Massachusetts, Amherst — The implantation of helium (He) atoms has significant implications for the surface morphological evolution and the near-surface structural evolution of plasma-facing components in nuclear fusion reactors. In tungsten (W), such interstitial He atoms are very mobile and aggregate to form clusters; the smaller of these clusters are mobile and their migration mediates the evolution of the surface morphology and the near-surface microstructure of the plasma-exposed material. In this presentation, we report results of a systematic atomic-scale analysis of the energetics and dynamics of mobile He clusters in near-surface W regions based on carefully parameterized many-body potentials. The analysis combines molecular-statics computations of the energies of structurally relaxed He-cluster configurations as a function of their distance from the surface with molecular-dynamics simulations of mobile cluster migration in the near-surface region. The cluster size n (ranging from 1 to 7 He atoms) and the surface crystallographic orientation are important parameters in the study. This atomic-scale analysis also is extended to the migration of small mobile He clusters near sinks other than surfaces, such as grain boundaries (GBs), with emphasis on GBs in near-surface regions.

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Date submitted: 11 Jul 2013

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